



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 04:07 AM UTC

PDB ID : 1SM7 / pdb_00001sm7
Title : Solution structure of the recombinant pronapin precursor, BnIb.
Authors : Pantoja-Uceda, D.; Palomares, O.; Bruix, M.; Villalba, M.; Rodriguez, R.; Rico, M.; Santoro, J.
Deposited on : 2004-03-08

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

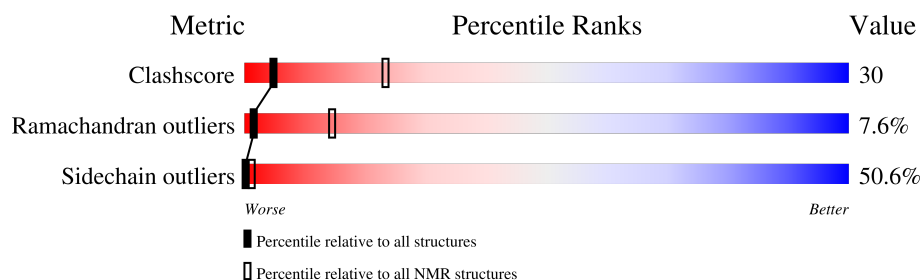
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	109	

2 Ensemble composition and analysis

This entry contains 19 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:24, A:43-A:71, A:81-A:109 (79)	0.87	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 6, 7, 10
2	2, 11, 12, 15, 17, 18
3	8, 14, 19
Single-model clusters	5; 9; 13; 16

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1725 atoms, of which 849 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called recombinant Ib pronapin.

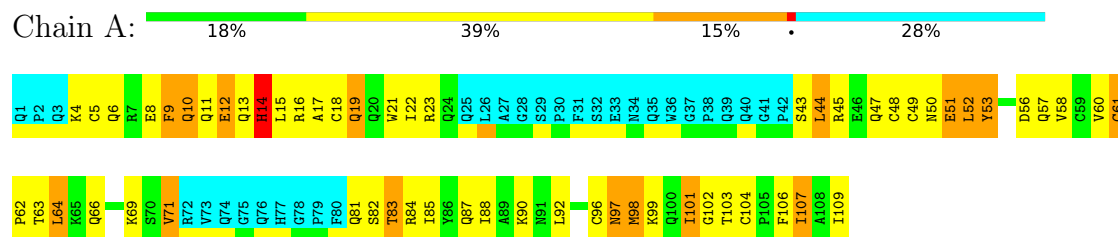
Mol	Chain	Residues	Atoms						Trace
1	A	109	Total	C	H	N	O	S	0
			1725	541	849	165	161	9	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: recombinant Ib pronapin

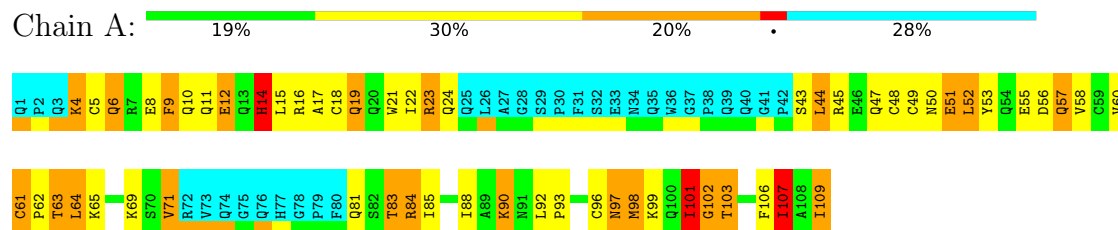


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

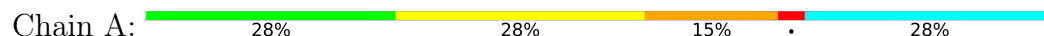
4.2.1 Score per residue for model 1 (medoid)

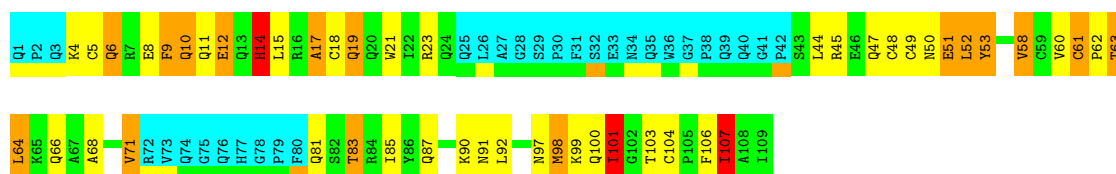
- Molecule 1: recombinant Ib pronapin



4.2.2 Score per residue for model 2

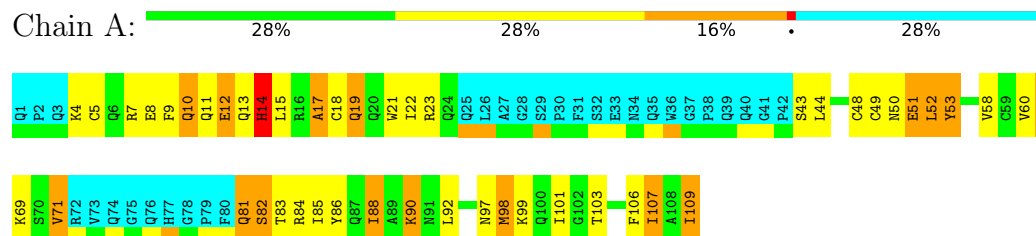
- Molecule 1: recombinant Ib pronapin





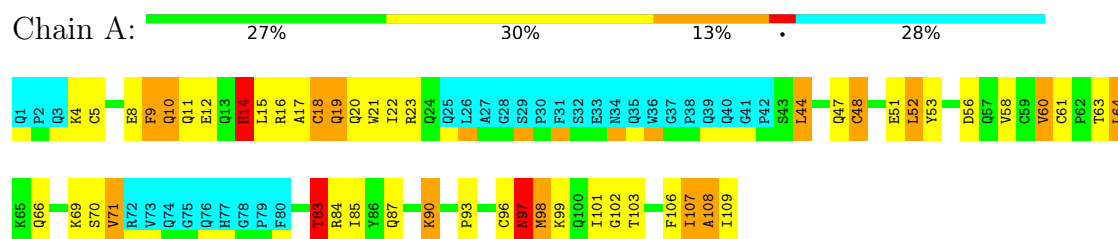
4.2.3 Score per residue for model 3

- Molecule 1: recombinant Ib pronapin



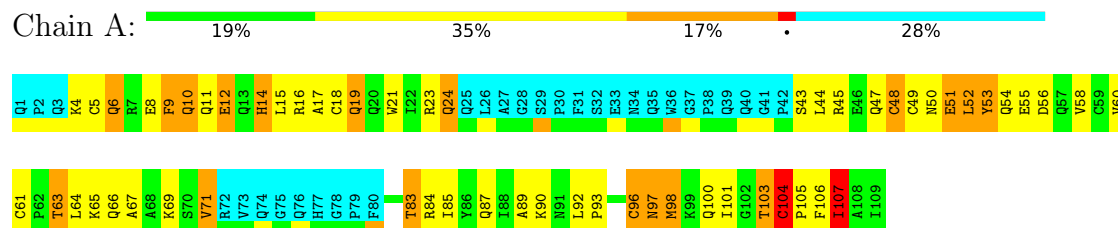
4.2.4 Score per residue for model 4

- Molecule 1: recombinant Ib pronapin



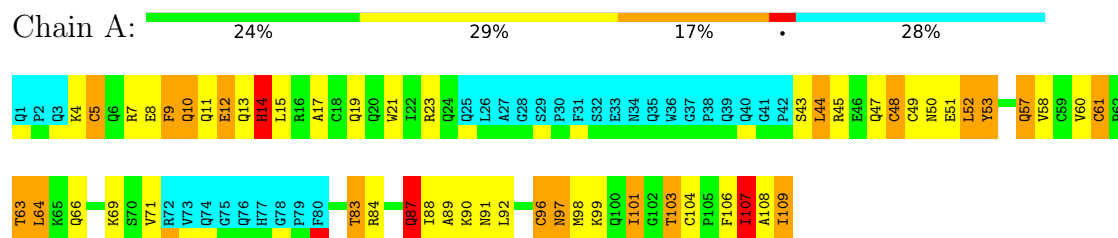
4.2.5 Score per residue for model 5

- Molecule 1: recombinant Ib pronapin



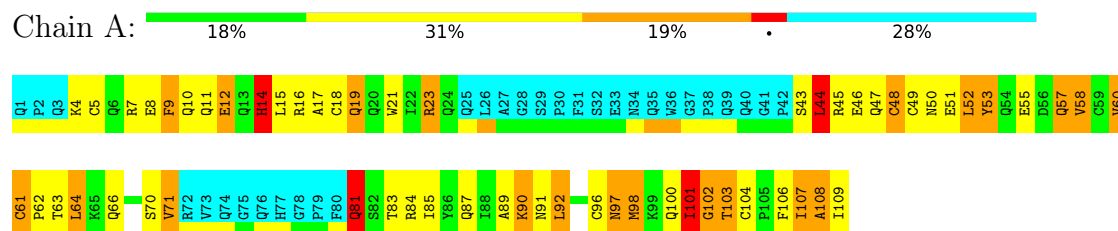
4.2.6 Score per residue for model 6

- Molecule 1: recombinant Ib pronapin



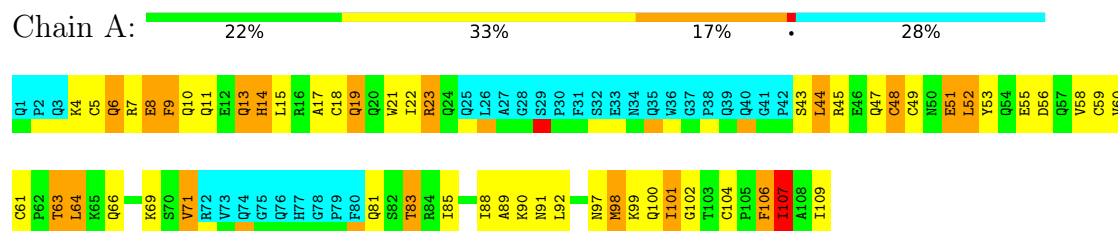
4.2.7 Score per residue for model 7

- Molecule 1: recombinant Ib pronapin



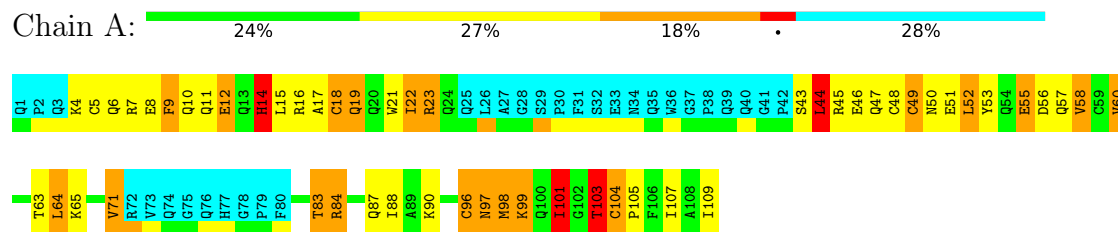
4.2.8 Score per residue for model 8

- Molecule 1: recombinant Ib pronapin



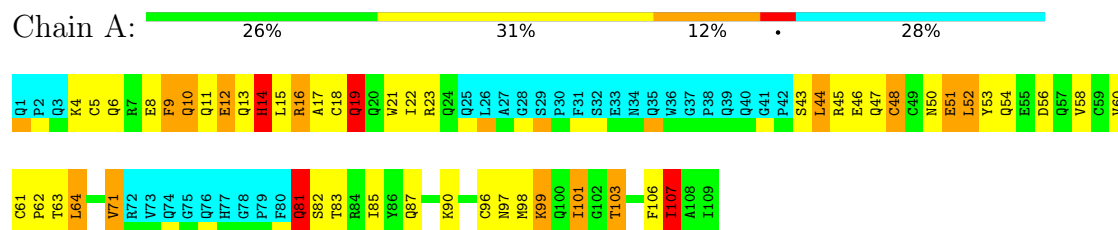
4.2.9 Score per residue for model 9

- Molecule 1: recombinant Ib pronapin



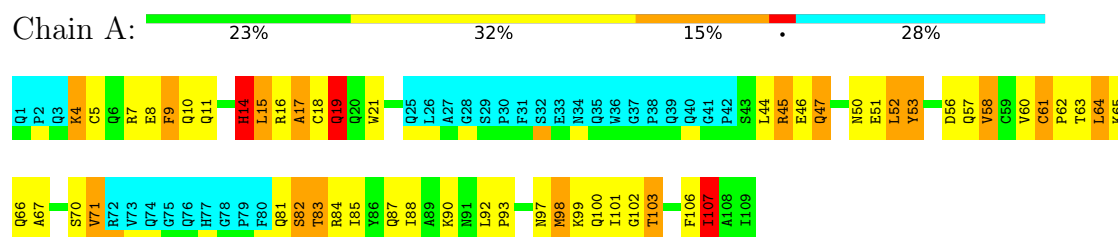
4.2.10 Score per residue for model 10

- Molecule 1: recombinant Ib pronapin



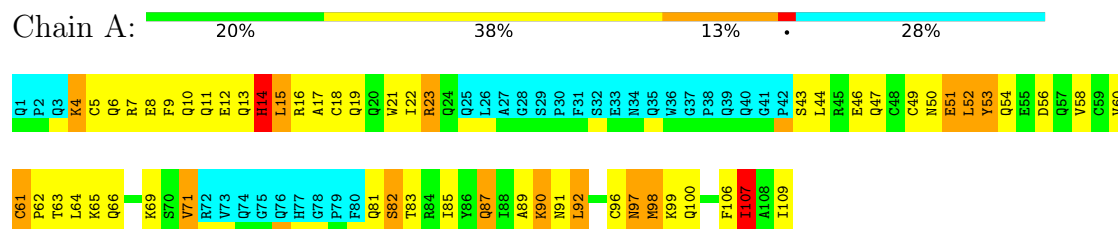
4.2.11 Score per residue for model 11

- Molecule 1: recombinant Ib pronapin



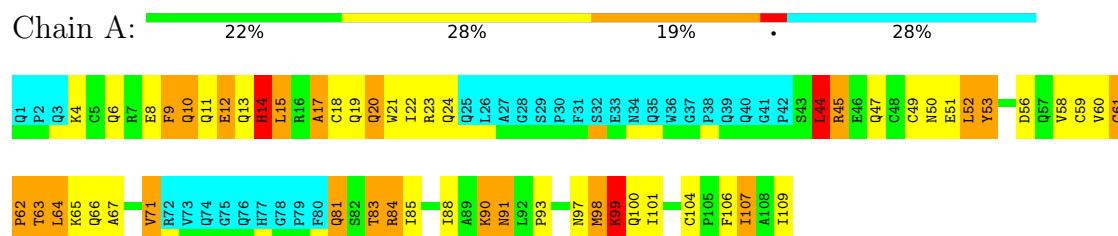
4.2.12 Score per residue for model 12

- Molecule 1: recombinant Ib pronapin



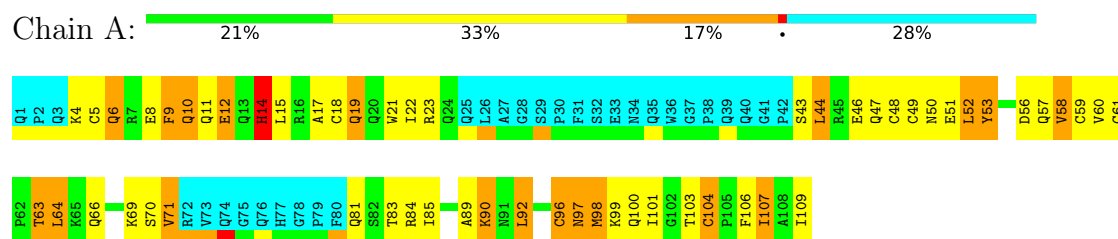
4.2.13 Score per residue for model 13

- Molecule 1: recombinant Ib pronapin



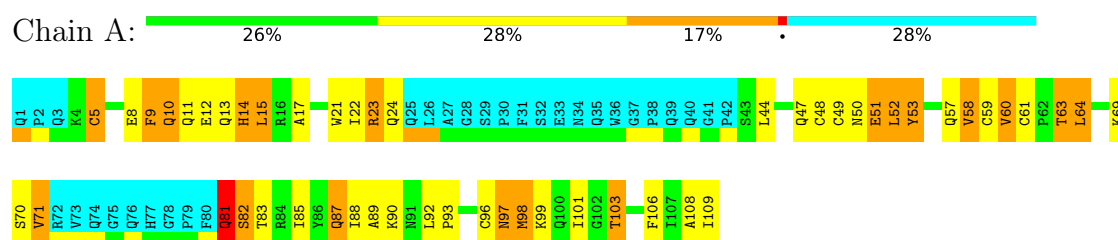
4.2.14 Score per residue for model 14

- Molecule 1: recombinant Ib pronapin



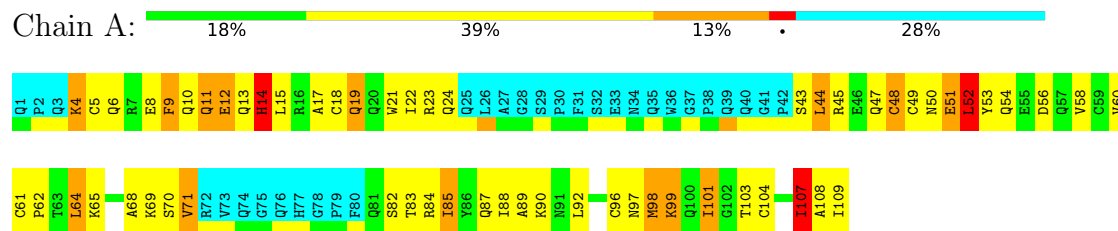
4.2.15 Score per residue for model 15

- Molecule 1: recombinant Ib pronapin



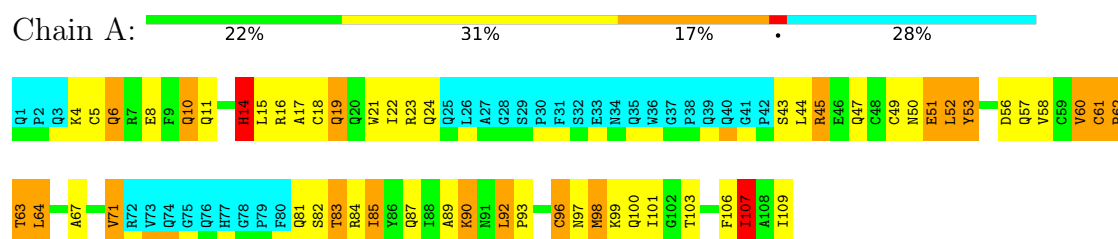
4.2.16 Score per residue for model 16

- Molecule 1: recombinant Ib pronapin



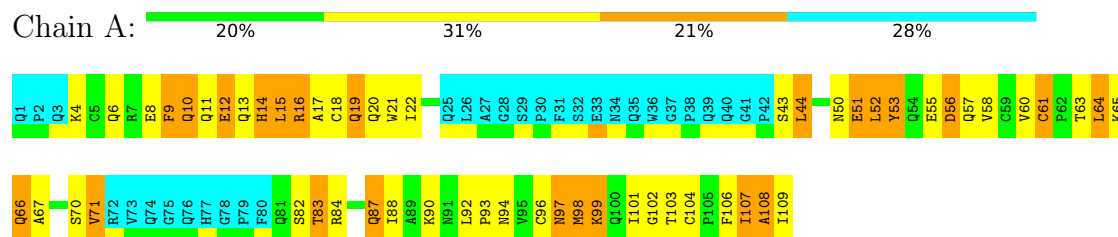
4.2.17 Score per residue for model 17

- Molecule 1: recombinant Ib pronapin



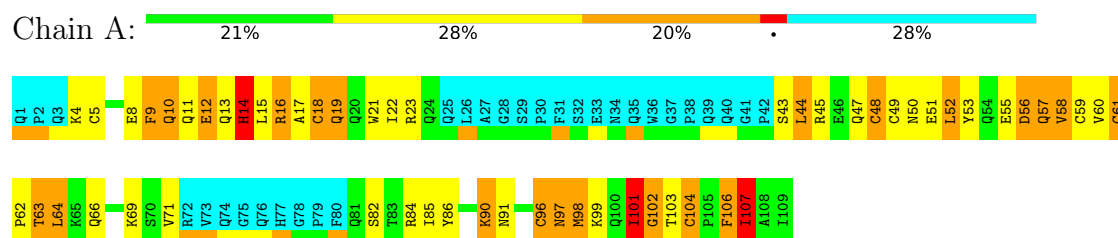
4.2.18 Score per residue for model 18

- Molecule 1: recombinant Ib pronapin



4.2.19 Score per residue for model 19

- Molecule 1: recombinant Ib pronapin



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, torsion angle dynamics*.

Of the 50 calculated structures, 19 were deposited, based on the following criterion: *structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
DIANA	structure solution	1.5
DIANA	refinement	1.5

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.91±0.06	0±0/652 (0.0± 0.0%)	1.42±0.14	3±3/876 (0.3± 0.3%)
All	All	0.91	0/12388 (0.0%)	1.42	50/16644 (0.3%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	GLN	OE1-CD-NE2	-8.49	114.11	122.60	10	3
1	A	105	PRO	N-CA-CB	8.01	108.04	102.35	9	2
1	A	13	GLN	OE1-CD-NE2	-7.50	115.10	122.60	10	5
1	A	87	GLN	OE1-CD-NE2	-6.97	115.63	122.60	6	3
1	A	66	GLN	OE1-CD-NE2	-6.85	115.75	122.60	5	1
1	A	88	ILE	N-CA-C	-6.58	106.38	112.96	3	1
1	A	81	GLN	CA-C-O	-6.30	114.41	120.90	13	3
1	A	4	LYS	CA-C-O	-6.18	114.53	120.90	11	2
1	A	101	ILE	CB-CA-C	6.10	116.89	111.71	10	1
1	A	62	PRO	CA-C-N	6.02	128.63	120.38	10	1
1	A	62	PRO	C-N-CA	6.02	128.63	120.38	10	1
1	A	19	GLN	OE1-CD-NE2	-6.01	116.59	122.60	10	2
1	A	24	GLN	OE1-CD-NE2	-5.91	116.69	122.60	5	1
1	A	4	LYS	CA-C-N	5.91	128.52	120.54	16	1
1	A	4	LYS	C-N-CA	5.91	128.52	120.54	16	1
1	A	62	PRO	N-CA-CB	5.83	109.02	102.60	16	4
1	A	63	THR	CA-CB-OG1	-5.58	101.22	109.60	13	1
1	A	52	LEU	CB-CA-C	5.58	118.40	109.02	16	1
1	A	91	ASN	OD1-CG-ND2	-5.58	117.02	122.60	13	1
1	A	64	LEU	CA-C-O	-5.49	114.70	120.63	13	1
1	A	82	SER	CA-C-O	-5.48	114.71	120.63	12	2
1	A	81	GLN	OE1-CD-NE2	-5.48	117.12	122.60	15	3
1	A	16	ARG	CA-C-O	-5.46	112.70	120.51	10	1
1	A	103	THR	CA-C-O	-5.41	114.49	120.60	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	47	GLN	CA-C-N	5.25	127.31	120.28	11	1
1	A	47	GLN	C-N-CA	5.25	127.31	120.28	11	1
1	A	85	ILE	N-CA-C	-5.17	107.11	111.56	16	1
1	A	99	LYS	CB-CA-C	5.15	118.61	111.51	16	1
1	A	8	GLU	CA-C-N	5.05	127.47	120.29	8	1
1	A	8	GLU	C-N-CA	5.05	127.47	120.29	8	1
1	A	101	ILE	N-CA-C	-5.03	106.75	111.48	10	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	643	637	636	38±9
All	All	12217	12103	12084	729

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LEU:HD23	1:A:64:LEU:HD12	0.96	1.35	4	5
1:A:22:ILE:HG21	1:A:85:ILE:HG23	0.87	1.46	3	1
1:A:52:LEU:HD23	1:A:64:LEU:CD1	0.85	2.01	1	15
1:A:52:LEU:HD13	1:A:53:TYR:N	0.83	1.87	1	18
1:A:17:ALA:HA	1:A:44:LEU:HD23	0.82	1.52	17	5
1:A:15:LEU:HD12	1:A:18:CYS:SG	0.81	2.15	18	4
1:A:17:ALA:HB1	1:A:44:LEU:CD2	0.80	2.06	9	3
1:A:71:VAL:HG11	1:A:85:ILE:HD12	0.80	1.54	13	7
1:A:23:ARG:HD3	1:A:71:VAL:HG22	0.80	1.53	2	2
1:A:14:HIS:C	1:A:15:LEU:HD23	0.78	2.04	9	14
1:A:17:ALA:HB1	1:A:44:LEU:HD23	0.77	1.55	14	11
1:A:52:LEU:HD23	1:A:64:LEU:HD11	0.76	1.57	14	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ALA:HB3	1:A:51:GLU:OE1	0.75	1.80	5	5
1:A:19:GLN:HB2	1:A:71:VAL:HG23	0.75	1.57	19	11
1:A:9:PHE:CG	1:A:63:THR:HG22	0.75	2.16	14	5
1:A:19:GLN:NE2	1:A:71:VAL:HG23	0.74	1.98	17	3
1:A:71:VAL:CG1	1:A:85:ILE:HD12	0.74	2.13	5	12
1:A:22:ILE:HD12	1:A:71:VAL:HG21	0.73	1.60	14	3
1:A:90:LYS:HD3	1:A:107:ILE:HG22	0.72	1.61	17	2
1:A:17:ALA:HB3	1:A:51:GLU:OE2	0.72	1.85	1	3
1:A:21:TRP:HB3	1:A:44:LEU:HD22	0.71	1.62	19	7
1:A:52:LEU:HD21	1:A:98:MET:CG	0.71	2.16	19	12
1:A:89:ALA:HA	1:A:92:LEU:HD12	0.71	1.62	14	9
1:A:52:LEU:HD13	1:A:52:LEU:C	0.71	2.09	19	15
1:A:90:LYS:HB2	1:A:107:ILE:HG22	0.70	1.63	3	1
1:A:90:LYS:HE3	1:A:109:ILE:OXT	0.70	1.87	14	1
1:A:84:ARG:NE	1:A:88:ILE:HD11	0.69	2.01	1	1
1:A:6:GLN:HG2	1:A:63:THR:HG23	0.69	1.64	1	2
1:A:52:LEU:HD21	1:A:98:MET:HG3	0.69	1.65	19	12
1:A:93:PRO:HB3	1:A:98:MET:HE2	0.69	1.62	5	4
1:A:52:LEU:HD22	1:A:60:VAL:HG22	0.69	1.63	3	11
1:A:21:TRP:CH2	1:A:88:ILE:HG22	0.69	2.23	13	5
1:A:52:LEU:CD2	1:A:60:VAL:HG22	0.67	2.20	3	17
1:A:19:GLN:HB3	1:A:67:ALA:HB1	0.67	1.65	13	1
1:A:19:GLN:HG3	1:A:67:ALA:HB1	0.67	1.65	11	1
1:A:23:ARG:CD	1:A:71:VAL:HG22	0.66	2.20	2	2
1:A:21:TRP:HB3	1:A:44:LEU:HD13	0.66	1.67	9	1
1:A:106:PHE:O	1:A:107:ILE:HG23	0.66	1.89	7	12
1:A:19:GLN:CB	1:A:71:VAL:HG23	0.66	2.20	7	10
1:A:21:TRP:HE1	1:A:92:LEU:HD11	0.66	1.51	11	7
1:A:9:PHE:CD2	1:A:63:THR:HG22	0.65	2.25	15	3
1:A:90:LYS:HG2	1:A:107:ILE:HG22	0.65	1.67	4	1
1:A:6:GLN:HA	1:A:63:THR:HG23	0.63	1.70	2	5
1:A:15:LEU:HD13	1:A:51:GLU:OE2	0.63	1.93	18	1
1:A:9:PHE:CE2	1:A:15:LEU:HD23	0.63	2.29	15	5
1:A:17:ALA:HB3	1:A:51:GLU:CD	0.62	2.19	13	3
1:A:14:HIS:O	1:A:15:LEU:HD23	0.62	1.94	19	7
1:A:64:LEU:HD13	1:A:98:MET:HE3	0.62	1.71	11	2
1:A:90:LYS:CD	1:A:107:ILE:HG22	0.62	2.25	12	2
1:A:22:ILE:HG22	1:A:23:ARG:NH1	0.61	2.10	12	1
1:A:19:GLN:O	1:A:71:VAL:HG23	0.61	1.95	16	2
1:A:17:ALA:HB1	1:A:44:LEU:HD21	0.61	1.73	6	3
1:A:19:GLN:CG	1:A:67:ALA:HB1	0.61	2.25	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:CYS:O	1:A:52:LEU:HD12	0.61	1.94	8	7
1:A:21:TRP:HH2	1:A:88:ILE:HG22	0.60	1.56	18	3
1:A:90:LYS:CB	1:A:106:PHE:CZ	0.60	2.85	1	1
1:A:52:LEU:HD21	1:A:60:VAL:HG22	0.59	1.74	10	4
1:A:20:GLN:NE2	1:A:44:LEU:HD21	0.59	2.11	13	1
1:A:107:ILE:HG23	1:A:109:ILE:H	0.59	1.57	16	1
1:A:87:GLN:HG3	1:A:109:ILE:HG22	0.59	1.75	18	2
1:A:84:ARG:O	1:A:88:ILE:HD12	0.58	1.98	16	1
1:A:19:GLN:HG2	1:A:67:ALA:HB1	0.58	1.73	18	2
1:A:106:PHE:CD1	1:A:109:ILE:HD11	0.58	2.34	15	1
1:A:90:LYS:CG	1:A:107:ILE:HG22	0.58	2.28	1	2
1:A:101:ILE:HD12	1:A:101:ILE:C	0.58	2.23	1	3
1:A:60:VAL:HG21	1:A:98:MET:O	0.57	2.00	12	6
1:A:52:LEU:HD22	1:A:52:LEU:C	0.57	2.24	12	5
1:A:49:CYS:HA	1:A:52:LEU:HD12	0.57	1.77	13	4
1:A:87:GLN:HG2	1:A:109:ILE:HD11	0.56	1.77	12	1
1:A:106:PHE:CE2	1:A:109:ILE:HD11	0.56	2.34	18	1
1:A:83:THR:HG22	1:A:84:ARG:N	0.56	2.14	18	6
1:A:21:TRP:NE1	1:A:92:LEU:HD11	0.56	2.15	11	1
1:A:108:ALA:C	1:A:109:ILE:HD12	0.56	2.25	16	1
1:A:109:ILE:OXT	1:A:109:ILE:HD12	0.56	2.01	1	1
1:A:19:GLN:CA	1:A:71:VAL:HG23	0.56	2.31	9	5
1:A:14:HIS:N	1:A:14:HIS:CD2	0.55	2.75	19	17
1:A:53:TYR:CE1	1:A:57:GLN:NE2	0.55	2.74	19	3
1:A:52:LEU:HD22	1:A:52:LEU:O	0.55	2.01	19	14
1:A:21:TRP:NE1	1:A:92:LEU:HD21	0.55	2.16	17	1
1:A:9:PHE:CD2	1:A:15:LEU:HD23	0.55	2.37	18	4
1:A:9:PHE:C	1:A:9:PHE:CD1	0.55	2.84	1	7
1:A:17:ALA:CB	1:A:44:LEU:HD23	0.55	2.31	5	9
1:A:87:GLN:HG2	1:A:109:ILE:OXT	0.55	2.02	6	1
1:A:21:TRP:CZ3	1:A:45:ARG:NH2	0.54	2.75	1	2
1:A:71:VAL:HG11	1:A:85:ILE:HG23	0.54	1.78	14	4
1:A:71:VAL:HG11	1:A:85:ILE:HG21	0.54	1.79	3	1
1:A:64:LEU:CD1	1:A:98:MET:HE3	0.54	2.32	7	3
1:A:53:TYR:CE2	1:A:98:MET:HA	0.54	2.37	18	9
1:A:19:GLN:HE21	1:A:71:VAL:HG23	0.54	1.60	17	2
1:A:93:PRO:HG2	1:A:107:ILE:HG21	0.54	1.80	13	1
1:A:61:CYS:SG	1:A:104:CYS:N	0.53	2.81	6	2
1:A:22:ILE:HD11	1:A:92:LEU:HD11	0.53	1.80	16	1
1:A:90:LYS:HG3	1:A:107:ILE:HG22	0.53	1.80	1	1
1:A:60:VAL:HG11	1:A:99:LYS:CB	0.53	2.34	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:TYR:CE2	1:A:98:MET:CB	0.52	2.92	7	6
1:A:19:GLN:HA	1:A:71:VAL:HG23	0.52	1.82	9	3
1:A:96:CYS:O	1:A:97:ASN:C	0.52	2.52	4	12
1:A:21:TRP:CB	1:A:44:LEU:HD13	0.52	2.34	9	2
1:A:99:LYS:CG	1:A:101:ILE:HG23	0.52	2.35	9	1
1:A:10:GLN:HA	1:A:14:HIS:CD2	0.52	2.40	1	17
1:A:21:TRP:CZ3	1:A:45:ARG:CZ	0.52	2.93	11	2
1:A:52:LEU:HD21	1:A:98:MET:SD	0.51	2.45	19	7
1:A:22:ILE:HG23	1:A:88:ILE:CG2	0.51	2.35	9	1
1:A:19:GLN:OE1	1:A:64:LEU:HD23	0.51	2.05	10	1
1:A:60:VAL:HG13	1:A:98:MET:HG3	0.51	1.83	18	5
1:A:52:LEU:HD11	1:A:98:MET:SD	0.51	2.46	6	3
1:A:61:CYS:SG	1:A:62:PRO:HA	0.51	2.47	19	5
1:A:9:PHE:CZ	1:A:63:THR:O	0.51	2.64	19	2
1:A:99:LYS:HG3	1:A:103:THR:HG22	0.50	1.83	10	1
1:A:52:LEU:CD2	1:A:98:MET:HE3	0.50	2.37	1	1
1:A:106:PHE:C	1:A:106:PHE:CD1	0.50	2.89	19	2
1:A:9:PHE:CD1	1:A:66:GLN:NE2	0.50	2.80	18	1
1:A:53:TYR:CE1	1:A:57:GLN:OE1	0.50	2.65	7	3
1:A:22:ILE:HG23	1:A:88:ILE:HG21	0.50	1.84	9	1
1:A:90:LYS:HD2	1:A:107:ILE:HG22	0.50	1.82	12	1
1:A:22:ILE:HB	1:A:71:VAL:HG21	0.50	1.82	18	1
1:A:9:PHE:CD2	1:A:55:GLU:OE1	0.49	2.65	9	1
1:A:104:CYS:SG	1:A:104:CYS:O	0.49	2.70	2	5
1:A:82:SER:O	1:A:86:TYR:CD1	0.49	2.65	19	1
1:A:93:PRO:HA	1:A:98:MET:SD	0.49	2.46	4	1
1:A:17:ALA:O	1:A:44:LEU:HD22	0.49	2.08	13	2
1:A:107:ILE:O	1:A:108:ALA:HB2	0.49	2.07	18	3
1:A:59:CYS:HA	1:A:63:THR:HG21	0.49	1.84	14	4
1:A:21:TRP:CH2	1:A:88:ILE:CG2	0.48	2.97	9	3
1:A:21:TRP:CE2	1:A:22:ILE:CG1	0.48	2.96	18	3
1:A:106:PHE:O	1:A:106:PHE:CG	0.48	2.67	7	2
1:A:51:GLU:O	1:A:51:GLU:HG3	0.48	2.08	16	1
1:A:68:ALA:O	1:A:71:VAL:HG12	0.48	2.08	16	2
1:A:98:MET:O	1:A:99:LYS:C	0.48	2.56	9	2
1:A:53:TYR:CE1	1:A:57:GLN:CD	0.48	2.91	19	1
1:A:93:PRO:CB	1:A:98:MET:HE2	0.48	2.36	5	1
1:A:89:ALA:CA	1:A:92:LEU:HD12	0.48	2.39	16	3
1:A:15:LEU:HD22	1:A:51:GLU:O	0.48	2.09	16	2
1:A:101:ILE:HG23	1:A:102:GLY:H	0.48	1.69	1	3
1:A:106:PHE:C	1:A:107:ILE:CG1	0.48	2.87	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:MET:SD	1:A:98:MET:N	0.47	2.87	4	1
1:A:18:CYS:HA	1:A:21:TRP:CD1	0.47	2.44	19	2
1:A:44:LEU:HD12	1:A:44:LEU:H	0.47	1.70	11	2
1:A:106:PHE:CD1	1:A:106:PHE:C	0.47	2.93	8	1
1:A:61:CYS:O	1:A:103:THR:HG21	0.46	2.09	1	5
1:A:21:TRP:CZ3	1:A:88:ILE:CG2	0.46	2.98	9	1
1:A:92:LEU:HB3	1:A:98:MET:HE1	0.46	1.86	8	1
1:A:60:VAL:CG1	1:A:99:LYS:HB2	0.46	2.41	9	1
1:A:71:VAL:HG13	1:A:85:ILE:HD12	0.46	1.88	2	1
1:A:5:CYS:SG	1:A:63:THR:HG21	0.46	2.51	6	1
1:A:14:HIS:CD2	1:A:14:HIS:N	0.46	2.84	18	2
1:A:92:LEU:N	1:A:93:PRO:CD	0.45	2.80	1	1
1:A:101:ILE:HG23	1:A:102:GLY:N	0.45	2.27	18	1
1:A:52:LEU:C	1:A:52:LEU:HD13	0.45	2.37	5	1
1:A:103:THR:HG23	1:A:104:CYS:N	0.45	2.26	19	2
1:A:21:TRP:CD1	1:A:44:LEU:HD22	0.45	2.46	10	1
1:A:55:GLU:O	1:A:56:ASP:CB	0.45	2.64	19	4
1:A:60:VAL:CG1	1:A:98:MET:HG3	0.45	2.41	19	5
1:A:99:LYS:HG2	1:A:101:ILE:HG23	0.45	1.89	9	1
1:A:90:LYS:HB3	1:A:106:PHE:CZ	0.45	2.46	1	1
1:A:90:LYS:HA	1:A:106:PHE:CZ	0.45	2.46	17	1
1:A:106:PHE:CD1	1:A:107:ILE:N	0.45	2.85	19	2
1:A:17:ALA:CA	1:A:44:LEU:HD23	0.44	2.42	1	2
1:A:52:LEU:HD21	1:A:98:MET:HE3	0.44	1.87	1	1
1:A:61:CYS:CB	1:A:62:PRO:HA	0.44	2.41	17	2
1:A:14:HIS:CD2	1:A:14:HIS:H	0.44	2.29	5	5
1:A:17:ALA:CB	1:A:44:LEU:HD21	0.44	2.41	9	2
1:A:5:CYS:HB2	1:A:58:VAL:HG12	0.44	1.89	15	1
1:A:94:ASN:OD1	1:A:107:ILE:HD13	0.44	2.13	18	1
1:A:57:GLN:NE2	1:A:57:GLN:N	0.44	2.65	19	1
1:A:53:TYR:CE2	1:A:98:MET:HB3	0.44	2.47	7	2
1:A:9:PHE:CD1	1:A:9:PHE:C	0.44	2.95	3	8
1:A:57:GLN:HE21	1:A:57:GLN:N	0.44	2.10	6	1
1:A:19:GLN:NE2	1:A:71:VAL:CG2	0.44	2.80	18	2
1:A:21:TRP:CE2	1:A:22:ILE:HG13	0.44	2.47	1	1
1:A:83:THR:CG2	1:A:84:ARG:N	0.43	2.81	1	5
1:A:19:GLN:CB	1:A:67:ALA:HB1	0.43	2.41	13	1
1:A:52:LEU:CD2	1:A:64:LEU:HD12	0.43	2.26	4	1
1:A:61:CYS:HB3	1:A:103:THR:HG22	0.43	1.90	18	1
1:A:61:CYS:HA	1:A:62:PRO:C	0.43	2.38	19	2
1:A:103:THR:O	1:A:104:CYS:C	0.43	2.61	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:PHE:CD2	1:A:63:THR:HB	0.43	2.48	11	1
1:A:21:TRP:CZ2	1:A:22:ILE:HG12	0.43	2.49	18	1
1:A:22:ILE:HG21	1:A:71:VAL:HG11	0.43	1.90	18	1
1:A:49:CYS:C	1:A:52:LEU:HD12	0.43	2.38	3	1
1:A:17:ALA:C	1:A:44:LEU:HD21	0.43	2.39	10	1
1:A:90:LYS:HB3	1:A:106:PHE:CE1	0.43	2.48	14	1
1:A:93:PRO:HB2	1:A:98:MET:HE1	0.43	1.89	4	1
1:A:93:PRO:CB	1:A:98:MET:CE	0.43	2.96	4	1
1:A:15:LEU:HD13	1:A:52:LEU:HB2	0.43	1.91	10	2
1:A:21:TRP:HA	1:A:44:LEU:HD13	0.43	1.91	13	2
1:A:9:PHE:CD1	1:A:10:GLN:N	0.43	2.87	18	1
1:A:9:PHE:CG	1:A:63:THR:HB	0.42	2.49	12	1
1:A:23:ARG:NH1	1:A:85:ILE:CD1	0.42	2.82	12	1
1:A:9:PHE:CE2	1:A:15:LEU:CD2	0.42	3.01	11	1
1:A:9:PHE:HZ	1:A:67:ALA:HB2	0.42	1.74	11	2
1:A:60:VAL:CG1	1:A:99:LYS:CB	0.42	2.97	9	1
1:A:71:VAL:HG11	1:A:85:ILE:CG2	0.42	2.45	19	2
1:A:106:PHE:O	1:A:109:ILE:HG23	0.42	2.15	3	2
1:A:56:ASP:O	1:A:60:VAL:HG23	0.42	2.14	17	3
1:A:62:PRO:O	1:A:65:LYS:CB	0.42	2.68	13	1
1:A:57:GLN:OE1	1:A:101:ILE:CG2	0.42	2.68	1	1
1:A:53:TYR:CZ	1:A:98:MET:HA	0.42	2.49	18	4
1:A:90:LYS:NZ	1:A:91:ASN:ND2	0.42	2.68	7	1
1:A:92:LEU:CB	1:A:93:PRO:HD3	0.42	2.44	17	2
1:A:17:ALA:HA	1:A:44:LEU:CD2	0.42	2.45	1	2
1:A:45:ARG:O	1:A:49:CYS:SG	0.42	2.77	1	1
1:A:90:LYS:HB3	1:A:106:PHE:CE2	0.42	2.49	1	1
1:A:17:ALA:CA	1:A:44:LEU:HD21	0.41	2.45	6	1
1:A:21:TRP:N	1:A:44:LEU:HD22	0.41	2.29	18	1
1:A:106:PHE:CD2	1:A:109:ILE:HD11	0.41	2.50	18	1
1:A:106:PHE:CD2	1:A:106:PHE:O	0.41	2.73	18	1
1:A:62:PRO:HA	1:A:104:CYS:SG	0.41	2.55	19	1
1:A:18:CYS:N	1:A:48:CYS:HB2	0.41	2.31	4	1
1:A:10:GLN:O	1:A:11:GLN:C	0.41	2.63	16	1
1:A:96:CYS:O	1:A:98:MET:SD	0.41	2.78	17	2
1:A:84:ARG:NE	1:A:88:ILE:CD1	0.41	2.80	1	1
1:A:87:GLN:CG	1:A:109:ILE:HG22	0.41	2.43	18	1
1:A:60:VAL:HA	1:A:64:LEU:HD12	0.41	1.92	3	1
1:A:52:LEU:C	1:A:52:LEU:HD22	0.41	2.40	6	1
1:A:55:GLU:HB3	1:A:59:CYS:CB	0.41	2.46	8	1
1:A:16:ARG:O	1:A:17:ALA:C	0.41	2.63	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:GLN:HA	1:A:71:VAL:CG2	0.41	2.46	14	3
1:A:15:LEU:HD21	1:A:55:GLU:OE2	0.41	2.15	5	1
1:A:90:LYS:CD	1:A:90:LYS:C	0.41	2.93	13	1
1:A:61:CYS:O	1:A:103:THR:CG2	0.41	2.69	1	1
1:A:93:PRO:CA	1:A:98:MET:SD	0.41	3.09	4	1
1:A:52:LEU:C	1:A:52:LEU:CD1	0.41	2.89	18	3
1:A:16:ARG:O	1:A:20:GLN:CG	0.41	2.69	18	1
1:A:21:TRP:CE2	1:A:22:ILE:HG12	0.41	2.51	18	1
1:A:101:ILE:C	1:A:101:ILE:HD12	0.41	2.41	19	1
1:A:55:GLU:O	1:A:59:CYS:SG	0.41	2.79	8	1
1:A:21:TRP:CH2	1:A:45:ARG:NH2	0.41	2.88	13	1
1:A:106:PHE:HD1	1:A:109:ILE:HD11	0.41	1.73	15	1
1:A:60:VAL:CG1	1:A:60:VAL:O	0.41	2.69	19	1
1:A:86:TYR:O	1:A:109:ILE:HD11	0.40	2.16	3	1
1:A:59:CYS:C	1:A:63:THR:OG1	0.40	2.64	19	1
1:A:89:ALA:CB	1:A:92:LEU:HD12	0.40	2.45	7	1
1:A:15:LEU:HD23	1:A:15:LEU:N	0.40	2.31	7	1
1:A:99:LYS:O	1:A:99:LYS:HG2	0.40	2.16	18	1
1:A:90:LYS:O	1:A:107:ILE:CG2	0.40	2.70	19	1
1:A:21:TRP:CE3	1:A:45:ARG:NH2	0.40	2.89	5	1
1:A:15:LEU:HD13	1:A:51:GLU:HG3	0.40	1.91	13	1
1:A:93:PRO:HG3	1:A:104:CYS:SG	0.40	2.57	5	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	78/109 (72%)	55±2 (70±3%)	18±3 (22±4%)	6±1 (8±2%)	1	14
All	All	1482/2071 (72%)	1036 (70%)	333 (22%)	113 (8%)	1	14

All 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	97	ASN	18
1	A	14	HIS	16
1	A	12	GLU	15
1	A	107	ILE	12
1	A	56	ASP	9
1	A	101	ILE	8
1	A	102	GLY	6
1	A	81	GLN	5
1	A	108	ALA	5
1	A	17	ALA	4
1	A	83	THR	3
1	A	44	LEU	3
1	A	82	SER	2
1	A	104	CYS	2
1	A	99	LYS	2
1	A	13	GLN	2
1	A	61	CYS	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	73/97 (75%)	36±4 (49±5%)	37±4 (51±5%)	0	1
All	All	1387/1843 (75%)	685 (49%)	702 (51%)	0	1

All 63 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	8	GLU	19
1	A	11	GLN	19
1	A	52	LEU	19
1	A	58	VAL	19
1	A	64	LEU	19
1	A	90	LYS	19
1	A	4	LYS	18
1	A	14	HIS	18
1	A	51	GLU	18

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Mol	Chain	Res	Type	Models (Total)
1	A	61	CYS	18
1	A	71	VAL	18
1	A	107	ILE	18
1	A	5	CYS	17
1	A	47	GLN	17
1	A	50	ASN	17
1	A	83	THR	17
1	A	98	MET	17
1	A	9	PHE	16
1	A	19	GLN	16
1	A	99	LYS	16
1	A	101	ILE	16
1	A	63	THR	15
1	A	12	GLU	14
1	A	43	SER	14
1	A	48	CYS	14
1	A	10	GLN	14
1	A	18	CYS	13
1	A	44	LEU	13
1	A	53	TYR	13
1	A	23	ARG	12
1	A	103	THR	12
1	A	6	GLN	11
1	A	66	GLN	11
1	A	87	GLN	11
1	A	16	ARG	10
1	A	69	LYS	10
1	A	49	CYS	10
1	A	45	ARG	10
1	A	100	GLN	9
1	A	84	ARG	8
1	A	109	ILE	8
1	A	82	SER	8
1	A	96	CYS	8
1	A	65	LYS	7
1	A	7	ARG	7
1	A	57	GLN	6
1	A	91	ASN	6
1	A	70	SER	6
1	A	46	GLU	6
1	A	24	GLN	5
1	A	60	VAL	5

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Mol	Chain	Res	Type	Models (Total)
1	A	22	ILE	5
1	A	15	LEU	5
1	A	13	GLN	4
1	A	104	CYS	4
1	A	81	GLN	4
1	A	92	LEU	4
1	A	55	GLU	2
1	A	106	PHE	2
1	A	85	ILE	2
1	A	97	ASN	1
1	A	20	GLN	1
1	A	54	GLN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided